

**Close out and Final report for
NASA Glenn Cooperative Agreement NCC3-650**

**Development, Implementation and Application of Micromechanical Analysis Tools for
Advanced High Temperature Composites**

This document contains the final report to the NASA Glenn Research Center (GRC) for the research project entitled "Development, Implementation, and Application of Micromechanical Analysis Tools for Advanced High-Temperature Composites." The research supporting this initiative has been conducted by Dr. Brett A. Bednarczyk, a Senior Scientist at OAI in Brookpark, Ohio from the period of August 1998 to March 2005.

Most of the work summarized herein involved development, implementation, and application of enhancements and new capabilities for NASA GRC's Micromechanics Analysis Code with Generalized Method of Cells (MAC/GMC) software package. When the project began, this software was at a low TRL (3-4) and at release version 2.0. Due to this project, the TRL of MAC/GMC has been raised to 7 and two new versions (3.0 and 4.0) have been released. The most important accomplishments with respect to MAC/GMC are: (1) a multi-scale framework has been built around the software, enabling coupled design and analysis from the global structure scale down to the micro fiber-matrix scale; (2) the software has been expanded to analyze smart materials; (3) state-of-the-art micromechanics theories have been implemented and validated within the code; (4) the damage, failure, and lifing capabilities of the code have been expanded from a very limited state to a vast degree of functionality and utility; and (5) the user flexibility of the code has been significantly enhanced. MAC/GMC is now the premier code for design and analysis of advanced composite and smart materials. It is a candidate for the 2005 NASA Software of the Year Award.

The work completed over the course of the project is summarized below on a year by year basis. All publications resulting from the project are listed at the end of this report.

1998-1999

A significant amount of progress was made towards providing improvements to and validation of micromechanical analysis tools for composite material systems of interest to NASA. The research for this project focused on the materials selection and design effort for NASA's Reusable Launch Vehicle (RLV) engine turbo pump housing. This effort, in cooperation with Boeing's Rocketdyne division, has helped narrow the field of metal matrix composite systems under consideration for this high thermal gradient application. In particular, the micromechanics analysis tool known as MAC/GMC was used to perform simulations that identified the source of premature failure in Nextel 610/copper-alloy composites which had been the frontrunner for the turbo pump housing. In order to perform these simulations, several tasks associated with this project were completed or undertaken. The constitutive model capabilities of MAC/GMC were extended to include the Freed-Walker viscoplastic model for copper and NARloy Z, as well as the Robinson viscoplastic model for NARloy Z. Studies conducted using these models, as well as the Bodner-Partom viscoplastic model, determined that the Robinson model for NARloy Z was

the most appropriate for the application at hand. The Robinson constitutive model allowed accurate simulation of the cool-down of the composite associated with its manufacturing. Results of packing arrangement studies indicated that high tensile stress concentrations can arise in the composite during the cool-down due to the close proximity of the small Nextel 610 fibers. Upon initiation of mechanical loading, these areas of high stress concentration are likely sites for damage and failure initiation and lead to composite failure at a much lower stress than is expected based on the strength of the fibers.

In order to simulate the behavior of different copper-alloy matrix composite laminates that could potentially fulfill the design requirements for the RLV application, the failure capabilities of MAC/GMC were extended. A recently developed debonding model that simulates local unloading of stresses in a composite was incorporated into the laminate theory capabilities of MAC/GMC, as was the ability to simulate laminate plies with discontinuous reinforcement. These new features were used to perform laminate ply arrangement studies for laminates with continuous Nextel 610 fibers, continuous silicon carbide fibers, and discontinuous and particulate aluminum oxide reinforcements. It was determined that a laminate consisting of an aluminum oxide particulate reinforced/copper-alloy core with $[0^\circ]$ and $[90^\circ]$ continuous silicon carbide fiber/copper-alloy layers has the potential to fulfill the design requirements for the RLV turbo pump housing.

Additional improvements were made to MAC/GMC through a cooperative effort with Dr. Carlos E. Orozco, a NASA Glenn summer faculty member. A new micromechanical procedure, known as the strain-compatible volume-average (SCVA) method, was incorporated into the MAC/GMC framework. This method was developed by Dr. Orozco, and by including coupling between normal and shear stresses in the formulation, it has the potential to allow more realistic and accurate simulations than previously possible with MAC/GMC for many applications.

With respect to the higher order theory for functionally graded materials (HOTFGM), work has focused on incorporating state of the art equation solvers into the model's computer codes. Especially in the context of time-dependent solutions, increased efficiency of the solution procedure is critical in order to perform desired studies. A demonstration version of the state of the art linear equation solver (developed via funding from NASA Langley) was incorporated into the computer code and decreased the execution times for HOTFGM by orders of magnitude. Subsequent to the delivery of the final version of this solver from NASA Langley, the solver will be incorporated into several distinct versions of the HOTFGM code, and meaningful simulations will be performed.

Finally, progress has been made regarding tasks associated with woven composites, the MAC/GMC unit cell library, and smart composites. The ability to model woven composites using transversely isotropic subcell material constitutive models has been made available to MAC/GMC users, and six new repeating unit cells have been added to the MAC/GMC unit cell library. Subroutines associated with analysis of smart composites have been written but still need to be merged with MAC/GMC.

1999–2000

A significant amount of progress was made towards providing improvements to and validation of micromechanical analysis tools for composite material systems of interest to NASA. Work on NASA's micromechanics analysis code with generalized method of cells (MAC/GMC) involved an extensive update of the entire code from the FORTRAN 77 standard to the FORTRAN 90 standard. This effort was completed and is significant in that the code's memory allocation is now dynamic. This has lifted restrictions that were in place previously that limited the size of problems that could be executed by the user. Further, the update to FORTRAN 90 has simplified data storage and data access in the code and has thus facilitated updates of and additions to the code's capabilities.

A major effort is also underway to reformulate completely MAC/GMC in terms of total quantities rather than rate-based quantities. That is, rather than calculating global stress and strain rates from local stress and strain rates and integrating both local and global rates to determine the total stresses and strains, MAC/GMC now integrates the local rates to determine the local stresses and strains. The global stresses and strains are then calculated directly from these local quantities. This improvement to the code allows incorporation of material models that employ implicit integration techniques, which are unconditionally stable and can improve execution times. One such implicitly integrated constitutive model has been incorporated into MAC/GMC, and an implicitly integrated visco-elasto-plastic constitutive model currently under development will be incorporated in the near future. In addition, the reformulation of MAC/GMC in terms of total quantities will enable the corporation of the classical incremental plasticity material constitutive model. This model is needed for continued support of NASA's Reusable Launch Vehicle (RLV) engine turbo pump housing development effort. This project shifted towards a material development effort in which the copper-based matrix alloy is being varied. In order to guide the development of this matrix alloy, a simple material constitutive model, such as classical incremental plasticity is highly desirable. This model's simplicity allows the yield and hardening properties of the modeled material to be easily varied in order to arrive at desirable composite behavior.

Progress has also been made in applying MAC/GMC to the longitudinal failure and transverse debonding behavior of continuous composites. The sub-models that were in place in MAC/GMC to simulate these phenomena were refined and applied to silicon carbide/titanium composites. Two NASA Technical Memoranda [1, 2] and two journal articles [3, 4] were published on these subjects.

A major breakthrough was achieved with respect to woven composites. A new two step approach in which homogenization occurs through the thickness of the woven composite prior to homogenization in the plane of the weave was developed for use in MAC/GMC. This approach allows significantly more accurate simulation of woven polymer matrix composites (which are the most common and useful type of woven composites) compared to the tradition one step homogenization approach previously employed in the context of MAC/GMC. A NASA Contractor Report that illustrates the viability of this new approach was published [5]. This new approach was slated to be fully coupled and automated within the MAC/GMC software.

In accordance with NASA Glenn Research Center's ISO 9000 certification, MAC/GMC was brought into compliance with the appropriate standards for low level software development. This involved documentation of procedures for updating and making additions to the code as well as the development of a large test suite with known results.

The micromechanical procedure known as the strain-compatible volume-average (SCVA) method, which eleven months ago showed great potential for enabling more accurate simulations within MAC/GMC, was fully evaluated. Via comparison with MAC/GMC's existing micromechanical procedure, the generalized method of cells (GMC), and finite element results, the SCVA method was shown to be deficient in terms of micro and macro accuracy. This method is being reworked (by its developer) and will be reevaluated in the future.

A great deal of progress was made with regard to the improvement and application of the higher order theory for functionally graded materials (HOTFGM). The state of the art sparse linear equation solver was incorporated into versions of NASA's HOTFGM code resulting in speed ups on the order of 7000 times. This improvement in HOTFGM's efficiency enabled the extensive investigation of the thermo-elastic response of an internally cooled silicon nitride plate. This work indicated the benefits of including cooling channels within ceramic turbine engine blades in order to lower the operating temperature. Further, this work led to the ability to model curved geometries using HOTFGM, significantly increasing the breadth of applicability of the model. A conference paper was prepared and presented on this work [6], and a NASA Technical Memorandum was published [7].

2000–2001

A great deal of progress was again accomplished. The incremental version of MAC/GMC was completed and brought into full functionality as the standard MAC/GMC version. This new version of the code was validated extensively and underwent significant debugging. Two new constitutive models, classical incremental plasticity and the implicit visco-elasto-plastic model, were successfully incorporated within MAC/GMC. A significant improvement was made to the incremental plasticity model as well. This enhancement allowed the model to simulate an inelastic material's response in a point-wise manner rather than the commonly employed simple bilinear approximation. The model was thus rendered considerably more accurate with respect to experimental results.

Substantial progress was made with respect to the inclusion of smart composites modeling capabilities within MAC/GMC. The ability to model smart composites was completed such that the code was capable of predicting the fully coupled electro-magneto-thermo-elastic response matrix of composites. This exceeded the goals for the year as magnetic effects were included in addition to the piezoelectric/pyroelectric effects that were proposed. Additional work involving more fully coupling the code's smart material capabilities with other existing capabilities (e.g., laminate analysis and arbitrary applied loading) was still pending.

A significant amount of attention was paid to extending MAC/GMC's failure analysis capabilities. New features were incorporated within MAC/GMC to allow any subcell to be subjected to several local and global failure models. In addition, these failure models were

coupled with the code's fatigue damage analysis and transverse debonding capabilities. The fatigue, failure, and debonding models were also extended to work in concert with the triply periodic (3D) and laminate analysis portions of MAC/GMC. This gives the user a great deal of generality for failure analysis of composite materials. These capabilities have been tested and validated. A NASA technical Memorandum [8] and a journal article [9] were published based on this work.

Significant attention was also paid to inclusion of the homogenized HOTFGM micromechanics approach within MAC/GMC. A doubly periodic (2D) version of the homogenized HOTFGM approach (now more commonly referred to as high-fidelity generalized method of cells, or HFGMC) [10] was incorporated within MAC/GMC and brought on-line. Additional work was needed to enable access to more of MAC/GMC's capabilities (e.g., damage analysis, transverse debonding, laminate analysis). Some verification work was done, but additional verification and exercising of HFGMC was needed.

Design and analysis of discontinuous composites was addressed through collaboration with a summer student at NASA GRC. Incorporation of the classical incremental plasticity constitutive model enabled the full evaluation of MAC/GMC with respect to modeling discontinuous composites. Support was provided to NASA regarding this effort. The resulting NASA report [11] indicated some deficiency in MAC/GMC's discontinuous composite capabilities. These deficiencies will be addressed through the incorporation of a triply periodic (3D) version of HFGMC.

Significant progress was also made with respect to the general maintenance, debugging, and support of MAC/GMC. The state of the code in terms of consistency, flow, and bugs was significantly improved. After much effort and considerable overhaul of the implicit visco-elasto-plastic constitutive model by the original developers, the model's MAC/GMC implementation was demonstrated. Work on new applications of HOTFGM resulted in a published journal paper [12]. Finally, the developed procedure for accurately modeling woven composites was more fully validated and documented in a conference paper [13] and a journal article [14].

2001–2002

Beginning in 2001, Dr. Bednarczyk began work on an additional project, which occupied approximately 80% of his time, while work on the project described herein was reduced to approximately 20%. This level of effort and funding continued through the remainder of the project.

A great deal of the year's effort went into maintenance, debugging, and support of MAC/GMC for the version 4.0 release of the software. The input format for the code was overhauled in order to make it more straightforward and user friendly. In addition, a new suite of example problems was compiled and documented. The MAC/GMC 4.0 User's Manual Volume 2 (Keywords Manual) [15] and Volume 3 (Example Problem Manual) [16] were written and published. Version 4.0 of MAC/GMC was released in December, 2002.

MAC/GMC's smart composite analysis capabilities were significantly enhanced. Arbitrary time-dependent mechanical, electrical, magnetic, and thermal loading was enabled for arbitrary smart composites, and smart composite laminates may also be analyzed with the code. These developments were documented in a NASA Contractor Report [17] and a journal article [18]. A shape memory alloy constitutive model was also incorporated within MAC/GMC.

2002–2003

A great deal of the year's effort again went toward maintenance, debugging, and support of MAC/GMC. The result was a strong state for the MAC/GMC software. The software was rendered well-documented, well-commented, and modular, while exhibiting a high level of interoperability. The ease of incorporating new capabilities into the code was significantly simplified thanks to the modular nature along with the fact that data objects were placed in a centrally-located modules.

MAC/GMC was applied to polymer matrix composites to some degree. The most notable additions to the code's capabilities in this realm involved the calculation of design allowables based on local stresses in the fiber and matrix. These types of allowables are often used for design and optimization of polymer matrix composites.

Fiber-matrix debonding capabilities were incorporated within the MAC/GMC HFGMC analysis module. An extensive study of debonding in titanium matrix composites was conducted using this new capability, resulting in a conference paper [19] and a journal article [20].

MAC/GMC was successfully utilized to analyze and aid in the design of shape memory titanium matrix composites, which were under consideration for several applications by the NASA GRC Materials Division. Many analyses were undertaken and compared to experimental data, and the results were summarized in five separate mini-reports over the last year. It was found that, while MAC/GMC can be calibrated based on a stress-free temperature to allow accurate prediction of the first-cycle plate response, an improved constitutive model for the titanium matrix would be needed in order to capture the ratcheting behavior.

2003–March 2005

The FEAMAC program, which now allows MAC/GMC to couple with the ABAQUS commercial finite element analysis software package was completed and released. This unique software allows micromechanics analyses to be performed (by the MAC/GMC core code) at points within a structural finite element analysis and is a major accomplishment of the project. A user's manual for FEAMAC has also been prepared and released (although not yet published as a NASA Technical Memorandum).

MAC/GMC was successfully applied to model the deformation and failure of polymer matrix composites and laminates. In particular, the progressive failure analysis capabilities enabled excellent agreement with test data from the world wide failure exercise. Additional work in this area is planned to more fully validate the progressive failure capabilities for polymer matrix composites.

Several triply-periodic versions of HFGMC were delivered to OAI from a contractor, and work was initiated to incorporate these within MAC/GMC. Initial work in this area resulted in the publication of a NASA Technical Memorandum [21]. Finally, a new, more accurate shape memory alloy constitutive model has been incorporated within MAC/GMC and verified.

Complete List of Publications and Presentations Resulting from Project

Journal Articles

1. Bednarczyk, B.A., Arnold, S.M., Aboudi, J., and Pindera, M.-J., 2004, "Local Field Effects in Titanium Matrix Composites Subject to Fiber-Matrix Debonding," *International Journal of Plasticity*, Vol. 20, 1707–1737.
2. Arnold, S.M., Bednarczyk, B.A., and Aboudi, J., 2004, "Analysis of Internally Cooled Structures Using a Higher Order Theory," *Computers and Structures*, Vol. 82, 659–688.
3. Bednarczyk, B.A. and Arnold, S.M., 2003, "Micromechanics-Based Modeling of Woven Polymer Matrix Composites," *AIAA Journal*, Vol. 41, 1788–1796.
4. Bednarczyk, B.A., 2003, "An Inelastic Micro/Macro Theory for Hybrid Smart/Metal Composites," *Composites: Part B*, Vol. 34, 175–197.
5. Bednarczyk, B.A., and Arnold, S.M., 2002, "Fully Coupled Micro/Macro Deformation, Damage, and Failure Prediction for SiC/Ti-15-3 Laminates," *Journal of Aerospace Engineering*, Vol. 14, No. 3, 74–83.
6. Bednarczyk, B.A., and Arnold, S.M., 2002, "Transverse Tensile and Creep Modeling of Continuously Reinforced Titanium Composites with Local Debonding," *International Journal of Solids and Structures*, Vol. 39, No. 7, 1987–2017.
7. Bednarczyk, B.A., 2001, "Discussion of 'Woven Fabric Composite Material Model with Material Non-Linearity for Non-Linear Finite Element Simulation' by Tabiei and Jiang," *International Journal of Solids and Structures*, Vol. 38, pp. 8585–8588.
8. Bednarczyk, B.A., and Arnold, S.M., 2001, "Micromechanics-Based Deformation and Failure Prediction for Longitudinally Reinforced Titanium Composites," *Composites Science and Technology*, Vol. 61, pp. 705–729.

NASA Publications

1. Arnold, S.M., Bednarczyk, B.A., and Aboudi, J., 2004, "Comparison of the Computational Efficiency of the Original versus Reformulated High-Fidelity Generalized Method of Cells," *NASA Technical Memorandum 213438*.
2. Bednarczyk, B.A., and Yarrington, P.W., 2004, "Elasto-Plastic Analysis of Tee Joints Using HOT-SMAC," *NASA Contractor Report 213067*.

3. Bednarczyk, B.A., and Arnold, S.M., 2002a, "MAC/GMC 4.0 User's Manual Volume 2: Keywords Manual," *NASA Technical Memorandum 212077/Vol 2*.
4. Bednarczyk, B.A., and Arnold, S.M., 2002b, "MAC/GMC 4.0 User's Manual Volume 3: Example Manual," *NASA Technical Memorandum 212077/Vol 3*.
5. Bednarczyk, B.A., 2002, "A Fully Coupled Micro/Macro Theory for Thermo-Electro-Magneto-Elasto-Plastic Composite Laminates," *NASA Contractor Report 211468*.
6. Bednarczyk, B.A., Arnold, S.M., and Lerch, B.A., 2001, "Fully Coupled Micro/Macro Deformation, Damage, and Failure Prediction for SiC/Ti-15-3 Laminates," *NASA Technical Memorandum 211343*.
7. Arnold, S.M., Bednarczyk, B.A., and Aboudi, J., 2001, "Thermo-Elastic Analysis of Internally Cooled Structures Using a Higher Order Theory," *NASA Technical Memorandum 210702*.
8. Bednarczyk, B.A., 2000, "Modeling Woven Polymer Matrix Composites With MAC/GMC," *NASA Contractor Report 210370*.
9. Bednarczyk, B.A., and Arnold, S.M., 2000, "A New Local Debonding Model with Application to the Transverse Tensile and Creep Behavior of Continuously Reinforced Titanium Composites," *NASA Technical Memorandum 210029*.
10. Arnold, S.M., Bednarczyk, B.A., Wilt, T.E., and Trowbridge, D., 2000, "Comprehensive Micromechanics-Analysis Code (MAC/GMC)," *NASA Tech Briefs*, Vol. 24, No. 2, pp. 39–40.
11. Bednarczyk, B.A., and Arnold, S.M., 2000, "A New Local Failure Model with Application to the Longitudinal Tensile Behavior of Continuously Reinforced Titanium Composites," *NASA Technical Memorandum 210027*.
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13. Arnold, S.M., Bednarczyk, B.A., Wilt, T.E., and Trowbridge, D., 1999, "Micromechanics Analysis Code with Generalized Method of Cells (MAC/GMC) User Guide: Version 3.0," *NASA Technical Memorandum 209070*.

Conferences and Invited Presentations

1. Bednarczyk, B.A., Arnold S.M., and Powers, L.M., 2005, "Micromechanics-Based FEA of Composite Structures," in *Proc. The Eleventh International Symposium on Plasticity*, January, Kauai, Hawaii.

2. Bednarczyk, B.A., 2005, "Multi-Scale Design and Analysis of Advanced Materials and Structures," Invited Lecture, United States Naval Academy Dept. Mechanical Engineering, March, Annapolis, Maryland.
3. Zhang, J., Bansal, Y., Bednarczyk, B.A., Collier, C.S., and Pindera, M.-J., 2004, "Analysis of Adhesively Bonded Composite Joints Using a Higher-Order Theory," in *Proc. 45th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference*, Palm Springs, California.
4. Bednarczyk, B.A., 2003, "An Inelastic Micro/Macro Theory for Hybrid Smart/Metal Composites," in *Proc. Tenth International Symposium on Plasticity*, July, Quebec City, Canada.
5. Bednarczyk, B.A., Yarrington, P.W., Collier, C.S., Arnold, S.M., Pindera, M.-J., and Aboudi, J., 2003, "Functionally Graded DRA for RLV Cryogenic Tanks," in *Proc. Fifth International Congress on Thermal Stresses and Related Topics*, June, Blacksburg, Virginia.
6. Yarrington, P.W., Collier, C.S., Bednarczyk, B.A., Arnold, S.M., Pindera, M.-J., and Aboudi, J., 2003, "Higher Order Theory—Structural/Micro Analysis Code (HOT-SMAC) Software for Thermo-Mechanical Analysis of FGMs," in *Proc. Fifth International Congress on Thermal Stresses and Related Topics*, June, Blacksburg, Virginia.
7. Shen, L., Lissenden, C.J., Bednarczyk, B.A., and Arnold, S.M., 2002, "Flow Surfaces for Fibrous Metal Matrix Composites Predicted by the Method of Cells," presented at the *39th Society of Engineering Science Technical Meeting*, October, State College, Pennsylvania.
8. Collier, C.S., Yarrington, P.W., Aboudi, J., Pindera, M.-J., Arnold, S.M., and Bednarczyk, B.A., 2002, "Higher Order Theory—Structural/Micro Analysis Code (HOT-SMAC) for Thermo-Mechanical Analysis of FGMs" in *Proc. MPIF 2002 International Conference on Functionally Graded Materials*, May, Denver, Colorado.
9. Bednarczyk, B.A., Arnold, S.M., Aboudi, J., and Pindera, M.-J., 2002, "Accurate Micro/Macro Field Simulation for Composites Subject to Fiber-Matrix Debonding Using HFGMC," in *Proc. 15th ASCE Engineering Mechanics Conference*, June, New York.
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11. Bednarczyk, B.A., Arnold, S.M., and Aboudi, J., 2000, "Modeling the Thermo-Elastic Behavior of an Internally Cooled Ceramic Plate Using HOTFGM," presented at *ICCE/7: The Seventh International Conference on Composites Engineering*, July, Denver, Colorado.

12. Bednarczyk, B.A., 2000, "Micromechanics-Based Multi-Scale Structural Analysis and Application-Driven Material Development," Invited Lecture, University of Virginia Dept. Civil Engineering Seminar Series, June, Charlottesville, Virginia.
13. Bednarczyk, B.A. and Arnold, S.M., 1999, "A New Local Failure/Debond Model with Application to the Tensile and Creep Behavior of Continuously Reinforced Composites," in *HITEMP Review 1999, NASA Conference Publication 208915*, Vol. 2, May, Cleveland, Ohio.
14. Bednarczyk, B.A. and Arnold, S.M., 1998, "Efficient Modeling of Micro Damage Events Leading to Macro Failure of Continuously Reinforced Composites," presented at *ICCE/5: The Fifth International Conference on Composites Engineering*, July, Las Vegas, Nevada.

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10. Aboudi, J., Pindera, M.-J., and Arnold, S.M., 2003, "Higher-Order Theory for Periodic Multiphase Materials with Inelastic Phases," *International Journal of Plasticity*, Vol. 19, 805–847.
11. Pahr, D.H. and Arnold S.M., "Applicability of the Generalized Method of Cells for Aligned Short Fiber Composites," *NASA Technical Memorandum 211165*.
12. Arnold, S.M., Bednarczyk, B.A., and Aboudi, J., 2004, "Analysis of Internally Cooled Structures Using a Higher Order Theory," *Computers and Structures*, Vol. 82, 659–688.
13. Bednarczyk, B.A. and Arnold, S.M., 2001, "Micromechanics-Based Modeling of Woven Polymer Matrix Composites," *42nd AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference and Exhibit, Seattle*. AIAA-2001-1567, A01-25288.
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